Maths for ML

Nipun Batra

IIT Gandhinagar

August 2, 2025

Maths for ML

1. Given a vector of ϵ, we can calculate $\sum \epsilon_i^2$ using $\epsilon^T \epsilon$

Maths for ML

1. Given a vector of ϵ, we can calculate $\sum \epsilon_i^2$ using $\epsilon^T \epsilon$

Maths for ML

1. Given a vector of ϵ, we can calculate $\sum \epsilon_i^2$ using $\epsilon^T \epsilon$

$$\epsilon = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \dots \\ \epsilon_N \end{bmatrix}_{N \times 1}$$

Maths for ML

1. Given a vector of ϵ, we can calculate $\sum \epsilon_i^2$ using $\epsilon^T \epsilon$

$$\epsilon = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \dots \\ \epsilon_N \end{bmatrix}_{N \times 1}$$

$$\epsilon^T = \begin{bmatrix} \epsilon_1, \epsilon_2, \dots, \epsilon_N \end{bmatrix}_{1 \times N}$$

Maths for ML

1. Given a vector of ϵ, we can calculate $\sum \epsilon_i^2$ using $\epsilon^T \epsilon$

$$\epsilon = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \dots \\ \epsilon_N \end{bmatrix}_{N \times 1}$$

$$\epsilon^T = \begin{bmatrix} \epsilon_1, \epsilon_2, \dots, \epsilon_N \end{bmatrix}_{1 \times N}$$

$$\epsilon^T \epsilon = \sum \epsilon_i^2$$

Maths for ML

2.

$$(AB)^T = B^T A^T$$

Maths for ML

2.

$$(AB)^T = B^T A^T$$

Maths for ML

2. $$(AB)^T = B^T A^T$$

3. For a scalar s
$$s = s^T$$

Maths for ML

4. Derivative of a scalar s wrt a vector θ

$$\theta = \begin{bmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_N \end{bmatrix}$$

$$\frac{\partial s}{\partial \theta} =$$

Maths for ML

4. Derivative of a scalar s wrt a vector θ

$$\theta = \begin{bmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_N \end{bmatrix}$$

$$\frac{\partial s}{\partial \theta} =$$

Maths for ML

4. Derivative of a scalar *s* wrt a vector θ

$$\theta = \begin{bmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_N \end{bmatrix}$$

$$\frac{\partial s}{\partial \theta} = \begin{bmatrix} \frac{\partial s}{\partial \theta_1} \\ \frac{\partial s}{\partial \theta_2} \\ \vdots \\ \frac{\partial s}{\partial \theta_N} \end{bmatrix}$$

Maths for ML

5. If A is a row-vector ($1 \times n$ matrix).
   and θ is a column-vector ($n \times 1$) matrix.
   and $A\theta$ is a scalar.

Example

$$\theta = \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}_{2\times 1}$$

$$A = \begin{bmatrix} A_1 & A_2 \end{bmatrix}_{1\times 2}$$

$$A\theta_{1\times 1} = A_1\theta_1 + A_2\theta_2$$

Maths for ML

$$\frac{\partial A\theta}{\partial \theta} = \begin{bmatrix} \frac{\partial}{\partial \theta_1}(A_1\theta_1 + A_2\theta_2) \\ \frac{\partial}{\partial \theta_2}(A_1\theta_1 + A_2\theta_2) \end{bmatrix} = \begin{bmatrix} A_1 \\ A_2 \end{bmatrix}_{2\times 1} = A^T$$

Maths for ML

6. Assume Z is a matrix of format $X^T X$, then $\frac{\partial}{\partial\theta}(\theta^T Z\theta) = 2Z^T\theta$

Maths for ML

6. Assume Z is a matrix of format $X^T X$, then $\frac{\partial}{\partial \theta}(\theta^T Z \theta) = 2Z^T \theta$

Maths for ML

6. Assume Z is a matrix of format $X^T X$, then $\frac{\partial}{\partial \theta}(\theta^T Z \theta) = 2Z^T \theta$

$$X = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

Maths for ML

6. Assume Z is a matrix of format $X^T X$, then $\frac{\partial}{\partial\theta}(\theta^T Z\theta) = 2Z^T\theta$

$$X = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

$$X^T = \begin{bmatrix} a & c \\ b & d \end{bmatrix}$$

Maths for ML

6. Assume Z is a matrix of format $X^T X$, then $\frac{\partial}{\partial\theta}(\theta^T Z\theta) = 2Z^T\theta$

$$X = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

$$X^T = \begin{bmatrix} a & c \\ b & d \end{bmatrix}$$

$$Z = X^T X = \begin{bmatrix} a^2 + c^2 & ab + cd \\ ab + cd & b^2 + d^2 \end{bmatrix}_{2\times 2}$$

Maths for ML

6. Assume Z is a matrix of format $X^T X$, then $\frac{\partial}{\partial\theta}(\theta^T Z\theta) = 2Z^T\theta$

$$X = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

$$X^T = \begin{bmatrix} a & c \\ b & d \end{bmatrix}$$

$$Z = X^T X = \begin{bmatrix} a^2 + c^2 & ab + cd \\ ab + cd & b^2 + d^2 \end{bmatrix}_{2\times 2}$$

Z has a property $Z_{ij} = Z_{ji} \implies Z^T = Z$

Maths for ML

Let

$$Z = X^T X = \begin{bmatrix} e & f \\ f & g \end{bmatrix}_{2\times 2}$$

Maths for ML

Let

$$Z = X^T X = \begin{bmatrix} e & f \\ f & g \end{bmatrix}_{2\times 2}$$

$$\theta = \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}_{2\times 1}$$

Maths for ML

Let

$$Z = X^T X = \begin{bmatrix} e & f \\ f & g \end{bmatrix}_{2\times 2}$$

$$\theta = \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}_{2\times 1}$$

$$\theta^T Z \theta = \begin{bmatrix} \theta_1 & \theta_2 \end{bmatrix}_{1\times 2} \begin{bmatrix} e & f \\ f & g \end{bmatrix}_{2\times 2} \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}_{2\times 1}$$

Maths for ML

Let

$$Z = X^T X = \begin{bmatrix} e & f \\ f & g \end{bmatrix}_{2\times 2}$$

$$\theta = \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}_{2\times 1}$$

$$\theta^T Z\theta = \begin{bmatrix} \theta_1 & \theta_2 \end{bmatrix}_{1\times 2} \begin{bmatrix} e & f \\ f & g \end{bmatrix}_{2\times 2} \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}_{2\times 1}$$

$$\theta^T Z\theta = \begin{bmatrix} \theta_1 & \theta_2 \end{bmatrix}_{1\times 2} \begin{bmatrix} e\theta_1 + f\theta_2 \\ f\theta_1 + g\theta_2 \end{bmatrix}_{2\times 1}$$

$$\theta^T Z\theta = e\theta_1^2 + 2f\theta_1\theta_2 + g\theta_2^2$$

The term $\theta^T Z\theta$ is a scalar.

Maths for ML

$$
\begin{aligned}
\frac{\partial}{\partial \theta}\theta^T Z\theta &= \frac{\partial}{\partial \theta}(e\theta_1^2 + 2f\theta_1\theta_2 + g\theta_2^2) \\
&= \begin{bmatrix} \frac{\partial}{\partial \theta_1}(e\theta_1^2 + 2f\theta_1\theta_2 + g\theta_2^2) \\ \frac{\partial}{\partial \theta_2}(e\theta_1^2 + 2f\theta_1\theta_2 + g\theta_2^2) \end{bmatrix} \\
&= \begin{bmatrix} 2e\theta_1 + 2f\theta_2 \\ 2f\theta_1 + 2g\theta_2 \end{bmatrix} = 2\begin{bmatrix} e & f \\ f & g \end{bmatrix}\begin{bmatrix} \theta_1 \\ \theta_1 \end{bmatrix}
\end{aligned}
$$

$$= 2Z\theta = 2Z^T\theta$$

Maths for ML: Matrix Rank[1]

- An *rxc* matrix as a set of *r* row vectors, each having *c* elements; or you can think of it as a set of *c* column vectors, each having *r* elements.

[1] Courtesy: https://stattrek.com/matrix-algebra/matrix-rank.aspx

Maths for ML: Matrix Rank[1]

- An *rxc* matrix as a set of *r* row vectors, each having *c* elements; or you can think of it as a set of *c* column vectors, each having *r* elements.
- The rank of a matrix is defined as (a) the maximum number of linearly independent column vectors in the matrix or (b) the maximum number of linearly independent row vectors in the matrix. Both definitions are equivalent.

[1] Courtesy: https://stattrek.com/matrix-algebra/matrix-rank.aspx

Maths for ML: Matrix Rank[1]

- An *rxc* matrix as a set of *r* row vectors, each having *c* elements; or you can think of it as a set of *c* column vectors, each having *r* elements.
- The rank of a matrix is defined as (a) the maximum number of linearly independent column vectors in the matrix or (b) the maximum number of linearly independent row vectors in the matrix. Both definitions are equivalent.
- If *r* is less than *c*, then the maximum rank of the matrix is *r*.

[1] Courtesy: https://stattrek.com/matrix-algebra/matrix-rank.aspx

Maths for ML: Matrix Rank[1]

- An *rxc* matrix as a set of *r* row vectors, each having *c* elements; or you can think of it as a set of *c* column vectors, each having *r* elements.
- The rank of a matrix is defined as (a) the maximum number of linearly independent column vectors in the matrix or (b) the maximum number of linearly independent row vectors in the matrix. Both definitions are equivalent.
- If *r* is less than *c*, then the maximum rank of the matrix is *r*.
- If *r* is greater than *c*, then the maximum rank of the matrix is *c*.

[1]Courtesy: https://stattrek.com/matrix-algebra/matrix-rank.aspx

Maths for ML: Matrix Rank

- Given a matrix A:

$$\begin{bmatrix} 0 & 1 & 2 \\ 1 & 2 & 1 \\ 2 & 7 & 8 \end{bmatrix}$$

Maths for ML: Matrix Rank

- Given a matrix A:

$$\begin{bmatrix} 0 & 1 & 2 \\ 1 & 2 & 1 \\ 2 & 7 & 8 \end{bmatrix}$$

- What is the rank?

Maths for ML: Matrix Rank

- Given a matrix A:

$$\begin{bmatrix} 0 & 1 & 2 \\ 1 & 2 & 1 \\ 2 & 7 & 8 \end{bmatrix}$$

- What is the rank?
- $r = c =$. Thus, rank is $<= 3$

Maths for ML: Matrix Rank

- Given a matrix A:

$$\begin{bmatrix} 0 & 1 & 2 \\ 1 & 2 & 1 \\ 2 & 7 & 8 \end{bmatrix}$$

- What is the rank?
- $r = c =$. Thus, rank is $<= 3$
- Row 3 can be written as: 3 times Row 1 + 2 times Row 1. Thus, Row 3 is linearly dependent on Row 1 and 2. Thus, rank(A)=2

Maths for ML: Matrix Rank

What is the rank of

$$X = \begin{bmatrix} 1 & 2 & 4 & 4 \\ 3 & 4 & 8 & 0 \end{bmatrix}$$

Maths for ML: Matrix Rank

What is the rank of

$$X = \begin{bmatrix} 1 & 2 & 4 & 4 \\ 3 & 4 & 8 & 0 \end{bmatrix}$$

Since X has fewer rows than columns, its maximum rank is equal to the maximum number of linearly independent rows. And because neither row is linearly dependent on the other row, the matrix has 2 linearly independent rows; so its rank is 2.

Maths for ML: Matrix Inverse

Suppose A is an $n \times n$ matrix. The inverse of A is another $n \times n$ matrix, denoted A^{-1}, that satisfies the following conditions.

$$\mathrm{A}\mathrm{A}^{-1} = \mathrm{A}^{-1}\mathrm{A} = \mathrm{I_n}$$

Maths for ML: Matrix Inverse

Suppose A is an $n \times n$ matrix. The inverse of A is another $n \times n$ matrix, denoted A^{-1}, that satisfies the following conditions.

$$\mathrm{A}\mathrm{A}^{-1} = \mathrm{A}^{-1}\mathrm{A} = \mathrm{I_n}$$

where $\mathrm{I_n}$ is the identity matrix.

Maths for ML: Matrix Inverse

Suppose A is an $n \times n$ matrix. The inverse of A is another $n \times n$ matrix, denoted A^{-1}, that satisfies the following conditions.

$$\mathrm{A}\mathrm{A}^{-1} = \mathrm{A}^{-1}\mathrm{A} = \mathrm{I}_\mathrm{n}$$

where I_n is the identity matrix.
Below, with an example, we illustrate the relationship between a matrix and its inverse.

Maths for ML: Matrix Inverse

Suppose A is an $n \times n$ matrix. The inverse of A is another $n \times n$ matrix, denoted A^{-1}, that satisfies the following conditions.

$$\mathrm{A}\mathrm{A}^{-1} = \mathrm{A}^{-1}\mathrm{A} = \mathrm{I_n}$$

where $\mathrm{I_n}$ is the identity matrix.
Below, with an example, we illustrate the relationship between a matrix and its inverse.

$$\begin{bmatrix} 2 & 1 \\ 3 & 4 \end{bmatrix} \begin{bmatrix} 0.8 & -0.2 \\ -0.6 & 0.4 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\begin{bmatrix} 0.8 & -0.2 \\ -0.6 & 0.2 \end{bmatrix} \begin{bmatrix} 2 & 1 \\ 3 & 4 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Maths for ML: Matrix Inverse

There are two ways to determine whether the inverse of a square matrix exists.

Maths for ML: Matrix Inverse

There are two ways to determine whether the inverse of a square matrix exists.

- If the rank of an $n \times n$ matrix is less than n, the matrix does not have an inverse.

Maths for ML: Matrix Inverse

There are two ways to determine whether the inverse of a square matrix exists.

- If the rank of an $n \times n$ matrix is less than n, the matrix does not have an inverse.
- When the determinant for a square matrix is equal to zero, the inverse for that matrix does not exist.

Maths for ML: Matrix Inverse

There are two ways to determine whether the inverse of a square matrix exists.

- If the rank of an $n \times n$ matrix is less than n, the matrix does not have an inverse.
- When the determinant for a square matrix is equal to zero, the inverse for that matrix does not exist.

Maths for ML: Matrix Inverse

There are two ways to determine whether the inverse of a square matrix exists.

- If the rank of an $n \times n$ matrix is less than n, the matrix does not have an inverse.
- When the determinant for a square matrix is equal to zero, the inverse for that matrix does not exist.

A square matrix that has an inverse is said to be nonsingular or invertible; a square matrix that does not have an inverse is said to be singular.

Maths for ML: Matrix Inverse

There are two ways to determine whether the inverse of a square matrix exists.

- If the rank of an $n \times n$ matrix is less than n, the matrix does not have an inverse.
- When the determinant for a square matrix is equal to zero, the inverse for that matrix does not exist.

A square matrix that has an inverse is said to be nonsingular or invertible; a square matrix that does not have an inverse is said to be singular.
Not every square matrix has an inverse; but if a matrix does have an inverse, it is unique.